



Fast Water Transport in CNTs: length dependence and entrane/exit effects

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Fast Water Transport in CNTs: length dependence and entrane/exit effects JENS HONORE WALTHER, TU Denmark, PETROS KOUMOUTSAKOS, ETH Zurich — Superfast water transport in carbon nanotube (CNT) membranes has been reported in experimental studies. We use Molecular Dynamics simulations to elucidate the mechanisms of water entry, exit and transport in 2 nm -diameter hydrophobic CNTs embedded in a hydrophilic membrane matrix. We demonstrate, for the first time, that under imposed pressures of the order of 1 bar, water entry into the CNT cavity and exit from the CNT end, can occur only on pre-wetted membranes. We conduct large scale simulations for up to 500 nm long CNTs and observe a previously unseen dependence of the flow enhancement rates on the CNT length. We relate the present findings to past computational and experimental studies, we discuss previous continuum assessments for this flow and propose underlying physical mechanisms.

☒ Prefer Oral Session
☐ Prefer Poster Session

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